Interpreting the Kustaanheimo–Stiefel transform in gravitational dynamics

Saha, P

Abstract: The Kustaanheimo–Stiefel (KS) transform turns a gravitational two-body problem into a harmonic oscillator, by going to four dimensions. In addition to the mathematical-physics interest, the KS transform has proved very useful in N-body simulations, where it helps to handle close encounters. Yet the formalism remains somewhat arcane, with the role of the extra dimension being especially mysterious. This paper shows how the basic transformation can be interpreted as a rotation in three dimensions. For example, if we slew a telescope from zenith to a chosen star in one rotation, we can think of the rotation axis and angle as the KS transform of the star. The non-uniqueness of the rotation axis encodes the extra dimension. This geometrical interpretation becomes evident on writing KS transforms in quaternion form, which also helps to derive concise expressions for regularized equations of motion.

DOI: https://doi.org/10.1111/j.1365-2966.2009.15437.x

Originally published at:
Saha, P (2009). Interpreting the Kustaanheimo–Stiefel transform in gravitational dynamics. Monthly Notices of the Royal Astronomical Society, 400(1):228-231.
DOI: https://doi.org/10.1111/j.1365-2966.2009.15437.x

Telescope Slew as a Kustaanheimo-Stiefel transformation

Prasenjit Saha

Institute for Theoretical Physics, University of Zürich,
Winterthurerstrasse 190, 8057 Zürich, Switzerland

ABSTRACT

The Kustaanheimo-Stiefel transformation turns a Kepler problem into a harmonic oscillator, by way of a rather mysterious extra dimension. Much has been written about it, to which this paper adds a small note of interpretation: the basic transformation can be visualized as a rotation in three dimensions. For example, if we slew a telescope from zenith to a chosen star in one rotation, we can think of the rotation axis and angle as the KS transform of the star. Moreover, the non-uniqueness of said rotation axis encodes the extra dimension. The result becomes evident on writing the KS transformation in quaternion form. Further unexpected connections with gates in quantum computing are also made.

Subject headings:

1. Introduction

The Kustaanheimo-Stiefel transformation is a remarkable relation between the two most important elementary problems in dynamics: under a transformation of coordinates and time, a Kepler problem changes into a harmonic oscillator. Especially noteworthy is that the collision singularity in the Kepler problem is transformed into a regular point. The name comes from the works by Kustaanheimo (1964) and Kustaanheimo & Stiefel (1965), while the book by Stiefel & Scheifele (1971), which is largely devoted to the KS transformation and its consequences, is perhaps the best known source. For a very short summary, see 'regularization' in Binney & Tremaine (2008). An important application of the KS transformation is in numerical orbit integration, where the singularity-removal is used to great advantage for simulating dense stellar systems with near collisions (Aarseth & Zare 1974a,b; Mikkola & Aarseth 1989, 1993; Jernigan & Porter 1989). Some recent papers also re-examine the formalism itself (Bartsch 2003; Waldvogel 2006).

For the Kepler problem in two dimensions there is a much simpler version of the KS transformation going back to Levi-Civita (1920). In the Levi-Civita transformation, the coordinate plane is read as the complex plane, and the complex square root of the coordinate becomes the transformed coordinate. The geometrical interpretation is clear: the complex phase gets halved. The KS transformation is also a kind of square root, but in four dimensions. One wonders how the geometrical interpretation generalizes.

It turns out that slewing a telescope is a convenient geometrical analogy. Suppose the telescope is at zenith, and we want to slew it to a particular star in one rotation. Normally we would simply move along a great circle from the zenith to the star. But we might prefer a different rotation (to avoid the full moon, say). For example, we could choose the midpoint on the above great circle and rotate about it by 180°. In any case, the chosen rotation axis and the rotation angle are effectively the KS transform of the star. This idea of rotation in three dimensions about a non-unique axis generalizes the idea of halving the phase in the Levi-Civita case.

This paper does not present any new mathematical results. However, it reformulates results from different places in the literature in a way that makes relations more intuitive, and especially makes the geometrical interpretation evident.

2. Quaternions and Rotation

Before considering KS theory, it is useful to review a concise algebraic way of specifying rotations in three dimensions, not often used in astrophysics but standard in computer graphics: quaternions.

Quaternions are a generalization of complex numbers. The $\sqrt{-1}$ of complex numbers is replaced by three unit quaternions $\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}$, such that

$$\boldsymbol{i}\boldsymbol{i} = \boldsymbol{j}\boldsymbol{j} = \boldsymbol{k}\boldsymbol{k} = -1. \tag{1}$$

Multiplication is non-commutative, with products given by

$$\boldsymbol{i}\boldsymbol{j} = -\boldsymbol{j}\boldsymbol{i} = \boldsymbol{k} \tag{2}$$

and so on. In other words, quaternions are sort of like a combination of dot and cross products in vector algebra. (Although historically quaternions came first, having been invented by none other than W.R. Hamilton of Hamilton's equations.)

A general quaternion has the form

$$\boldsymbol{A} = A_0 + A_x\boldsymbol{i} + A_y\boldsymbol{j} + A_z\boldsymbol{k} \tag{3}$$

where we will call A_0 the real part. A quaternion with no real part is effectively a vector.

In analogy with complex numbers, we will use the following notation for quaternion conjugates and absolute values.

$$\begin{aligned} \mathrm{re}\,[\boldsymbol{A}] &\equiv A_0 \\ \boldsymbol{A}^* &\equiv \boldsymbol{A} = A_0 - A_1\boldsymbol{i} - A_2\boldsymbol{j} - A_3\boldsymbol{k} \\ A^2 &\equiv \boldsymbol{A}^*\boldsymbol{A} = A_0^2 + A_1^2 + A_2^2 + A_3^2 \end{aligned} \tag{4}$$

It is easy to see that $\mathrm{re}\,[\boldsymbol{A}^*] = \mathrm{re}\,[\boldsymbol{A}]$ and $(\boldsymbol{AB})^* = \boldsymbol{B}^*\boldsymbol{A}^*$, and as a result

$$\mathrm{re}\,[\boldsymbol{AB}] = \mathrm{re}\,[\boldsymbol{B}^*\boldsymbol{A}^*] = \mathrm{re}\,[\boldsymbol{BA}]\,. \tag{5}$$

Rotation in quaternion notation is beautifully concise. Say we want to rotate a vector $\boldsymbol{r}$ by angle ω about a unit vector $\boldsymbol{n}$. Using quaternion algebra the rotation is simply

$$\boldsymbol{R}^*\boldsymbol{r}\boldsymbol{R} \tag{6}$$

where

$$\boldsymbol{R} = \cos\tfrac{1}{2}\omega + \sin\tfrac{1}{2}\omega\,\boldsymbol{n}. \tag{7}$$

(If $\boldsymbol{n}$ is not a unit vector there is a scalar multiplication by n^2.) Unlike the equivalent expression using Euler angles, the expression (6) has no coordinate singularities (or “gimbal lock”) and as a result is numerically more stable, which explains its popularity in computer graphics.

It is possible to represent quaternions as matrices (though not necessary, even for numerical work). A familiar representation is in terms of Pauli matrices

$$\boldsymbol{i} = i\sigma_1 \qquad \boldsymbol{j} = -i\sigma_2 \qquad \boldsymbol{k} = i\sigma_3. \tag{8}$$

Pauli matrices are most important as operators on quantum two-state systems (being Hermitian, whereas quaternions are anti-Hermitian). In recent years the most exciting two-state quantum systems have been Qbits in quantum computing. It turns out that expressions of the type (6) appear in the description of quantum-computing gates (see Mermin 2007, who also provides a derivation of essentially the above three-dimensional rotation formula).

3. The Kustaanheimo-Stiefel transformation

Let

$$\boldsymbol{q} = x\boldsymbol{i} + y\boldsymbol{j} + z\boldsymbol{k} \tag{9}$$

denote a point in space. The KS transform of $\boldsymbol{q}$ is the quaternion

$$\boldsymbol{Q} = Q_0 + Q_x\boldsymbol{i} + Q_y\boldsymbol{j} + Q_z\boldsymbol{k} \tag{10}$$

while the transformation itself is

$$\boldsymbol{q} = \boldsymbol{Q}^*\boldsymbol{k}\,\boldsymbol{Q}. \tag{11}$$

A solution for $\boldsymbol{Q}$ is

$$\boldsymbol{Q}^I = \frac{x\boldsymbol{i} + y\boldsymbol{j} + Z\boldsymbol{k}}{\sqrt{2Z}} \qquad Z \equiv z + \sqrt{x^2+y^2+z^2} \tag{12}$$

as is easily verified by multiplication, following the quaternion rules. But $\boldsymbol{Q}^{\boldsymbol{I}}$ is not unique, because changing to

$$\boldsymbol{Q} = (\cos\psi + \sin\psi\,\boldsymbol{k})\,\boldsymbol{Q}^I \tag{13}$$

leaves Equation (11) invariant. Thus ψ behaves like a gauge.

Everything so far is already in the literature. The new result in this paper is that we can readily visualize $\boldsymbol{Q}$, including its non-uniqueness.

Comparing (11) and (6), it is evident that $\boldsymbol{Q}$ is a rotator that takes the z axis to $\boldsymbol{q}$. To visualize $\boldsymbol{Q}$, let us rewrite $\boldsymbol{q}$ as

$$\boldsymbol{q} = r(\sin\theta\cos\phi\,\boldsymbol{i} + \sin\theta\sin\phi\,\boldsymbol{j} + \cos\theta\,\boldsymbol{k}) \tag{14}$$

where r, θ, ϕ are the usual polar coordinates. Rewriting $\boldsymbol{Q}^{\boldsymbol{I}}$ in the solution (12) and simplifying, we have

$$\boldsymbol{Q}^I = \sqrt{r}(\sin\tfrac{1}{2}\theta\cos\phi\,\boldsymbol{i} + \sin\tfrac{1}{2}\theta\sin\phi\,\boldsymbol{j} + \cos\tfrac{1}{2}\theta\,\boldsymbol{k}). \tag{15}$$

In other words, the direction of $\boldsymbol{Q}^{\boldsymbol{I}}$ is halfway along the great circle from $\boldsymbol{k}$ to $\boldsymbol{q}$. From (7) we see the rotation angle ω would be π. Now let us apply the gauge transformation (13) with $\psi = \pi$. This gives

$$\boldsymbol{Q}^{II} = \sqrt{r}(\cos\tfrac{1}{2}\theta - \sin\tfrac{1}{2}\theta\sin\phi\,\boldsymbol{i} + \sin\tfrac{1}{2}\theta\cos\phi\,\boldsymbol{j}) \tag{16}$$

Now the implied rotation is by θ, about an axis perpendicular to both $\boldsymbol{k}$ and $\boldsymbol{q}$. In general, $\boldsymbol{Q}$ could be anywhere on the great circle joining $\boldsymbol{Q}^{\boldsymbol{I}}$ and $\boldsymbol{Q}^{\boldsymbol{II}}$. Whence comes the telescope-slewing metaphor of the title.

An interesting special case is $\phi = 0$, which gives $\boldsymbol{q} = r(\cos\theta\,\boldsymbol{k} + \sin\theta\,\boldsymbol{i})$ and $\boldsymbol{Q}^{\boldsymbol{I}} = \sqrt{r}(\cos\frac{1}{2}\theta\,\boldsymbol{k} + \sin\frac{1}{2}\theta\,\boldsymbol{i})$. Then $\boldsymbol{Q}^{\boldsymbol{I}}$ is effectively the complex square root of $\boldsymbol{q}$ (we need to read $\boldsymbol{k}$ as the real axis and $\boldsymbol{i}$ as the imaginary axis). In other words, the planar case can be reduced to the Levi-Civita transformation by a suitable gauge.

That $\boldsymbol{Q}$ represents a rotation and shrinking/stretching of $\boldsymbol{q}$ and that the rotation axis is not unique in three dimensions is also noted by Bartsch (2003) though not so explicitly as here.

4. Hamiltonians and regularization

So far we have just discussed geometry, but of course the real significance of the KS transformation is dynamics, which we now consider. Let

$$\boldsymbol{p} = p_x\boldsymbol{i} + p_y\boldsymbol{j} + p_z\boldsymbol{k} \tag{17}$$

be the canonical momentum conjugate to $\boldsymbol{q}$. We seek

$$\boldsymbol{P} = P_0 + P_x\boldsymbol{i} + P_y\boldsymbol{j} + P_z\boldsymbol{k} \tag{18}$$

that will be canonically conjugate to $\boldsymbol{Q}$. Let us write

$$\mathrm{re}\,[\boldsymbol{p}^* d\boldsymbol{q}] = \mathrm{re}\,[\boldsymbol{p}^*\, d\boldsymbol{Q}^*\, \boldsymbol{k}\boldsymbol{Q}] + \mathrm{re}\,[\boldsymbol{p}^*\boldsymbol{Q}^*\boldsymbol{k}\, d\boldsymbol{Q}] \tag{19}$$

Using the identity (5) we can rewrite the middle term as $\mathrm{re}\,[\boldsymbol{Q}^*(-\boldsymbol{k})\, d\boldsymbol{Q}\, \boldsymbol{p}]$. Since $\boldsymbol{p}^* = -\boldsymbol{p}$ the term becomes $\mathrm{re}\,[\boldsymbol{Q}^*\boldsymbol{k}\, d\boldsymbol{Q}\, \boldsymbol{p}^*]$. Then using (5) again the term becomes $\mathrm{re}\,[\boldsymbol{p}^*\boldsymbol{Q}^*\boldsymbol{k}\, d\boldsymbol{Q}]$. Thus we have

$$\mathrm{re}\,[\boldsymbol{p}^* d\boldsymbol{q}] = 2\,\mathrm{re}\,[\boldsymbol{p}^*\boldsymbol{Q}^*\boldsymbol{k}\, d\boldsymbol{Q}] \tag{20}$$

Now if we define

$$\boldsymbol{P} = -2\boldsymbol{k}\boldsymbol{Q}\boldsymbol{p} \tag{21}$$

we have

$$\mathrm{re}\,[\boldsymbol{p}^* d\boldsymbol{q}] = \mathrm{re}\,[\boldsymbol{P}^* d\boldsymbol{Q}] \tag{22}$$

which is to say, $\boldsymbol{p}\cdot d\boldsymbol{q} = \boldsymbol{P}\cdot d\boldsymbol{Q}$. Provided the Hamiltonian depends on $\boldsymbol{P}, \boldsymbol{Q}$ only through $\boldsymbol{p}, \boldsymbol{q}$ and not on the gauge ψ, the transformation $(\boldsymbol{P}, \boldsymbol{Q}) \to (\boldsymbol{p}, \boldsymbol{q})$ is canonical.

To get an explicit expression for $\boldsymbol{p}$, we multiply (21) on the left by $\boldsymbol{Q}\boldsymbol{k}$, obtaining

$$\boldsymbol{p} = \frac{\boldsymbol{Q}^*\boldsymbol{k}\boldsymbol{P}}{2Q^2}. \tag{23}$$

Note that while we have to be careful about the order of multiplication when $\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}$ are involved, real numbers like Q^2 commute with everything. Since $\boldsymbol{p}$ has no real part, $\mathrm{re}\,[\boldsymbol{Q}^*\boldsymbol{k}\boldsymbol{P}] = 0$ identically. We can think of it as a formal constant of motion resulting from invariance with respect to ψ.

That $\boldsymbol{P}$ (as defined in Equation 21, or equivalently) completes a canonical transformation a standard part of KS theory, but the derivation of the canonical condition using quaternion identities appears to be new. The remainder of this section is also in the literature, though again not all in the same place.

Let us now write the Kepler Hamiltonian

$$H = \tfrac{1}{2}p^2 - 1/q^2 \tag{24}$$

in terms of KS variables. Multiplying each of (11) and (21) by its quaternion conjugate, we have

$$q^2 = Q^4, \qquad P^2 = 4p^2Q^2 \tag{25}$$

and substituting these gives

$$H = \tfrac{1}{8}P^2/Q^2 - 1/Q^2. \tag{26}$$

Next we introduce a fictitious time variable s, related to t by

$$dt = Q^2\, ds. \tag{27}$$

Since Q^2 is the radial distance in the Kepler problem, (27) is nothing but Kepler's equation, and s is the eccentric anomaly. Under this time-transformation (known as the Poincaré time transformation), the Hamiltonian changes

$$\Gamma = Q^2(H - E) = \tfrac{1}{8}P^2 - EQ^2 \tag{28}$$

with E being the constant initial value of H. The time-transformed Hamiltonian Γ is zero along a trajectory, though its partial derivatives will not be zero.

The transformed Hamiltonian Γ is remarkable indeed. For $E < 0$ (bound orbits) it is a harmonic oscillator. Since $\boldsymbol{Q}$ has four components, Γ is like a mass on an isotropic spring in four Euclidean dimensions. Thus the well-known fact that the bound Kepler problem has a dynamical $O(4)$ symmetry. For the unbound case, the symmetry group is different: formally the Lorentz group, but with a physical meaning completely different from special relativity. And—perhaps most importantly—Hamilton's equations for Γ are well-behaved even at $Q = 0$ (a collision). This is known as regularization and was perhaps the original motivation for KS theory.

KS regularization is exploited in N-body work on dense stellar systems, where the dynamics can be expressed as coupled Keplerian systems. KS variables are used for each Keplerian system, which becomes trivially integrable, while the couplings are treated as perturbations. The time transformation does not even need to be exactly as in (27), provided the time variable stretches as Q^2 in the collision limit. One only needs to compute the perturbation terms in the differential equations in terms of KS variables. This is fairly straightforward. For example, if there is an external force $\dot{\boldsymbol{p}}_{\rm ext}$, the effect on $\boldsymbol{P}$ follows trivially from (21) as

$$\dot{\boldsymbol{P}}_{\rm ext} = -2\boldsymbol{k}\boldsymbol{Q}\,\dot{\boldsymbol{p}}_{\rm ext}. \tag{29}$$

Derivatives of Hamiltonian terms with respect to $\boldsymbol{P}$ and $\boldsymbol{Q}$ will also be required. Two useful derivatives with respect to $\boldsymbol{Q}$ and $\boldsymbol{P}$ are as follows. The gradient

$$\nabla_{\boldsymbol{Q}}\, q = 2\boldsymbol{Q} \tag{30}$$

follows immediately from (25). Slightly more subtle is the gradient $\nabla_{\boldsymbol{P}}\,\mathrm{re}\,[\boldsymbol{P}^*\boldsymbol{A}] = \boldsymbol{A}$, from which

$$\nabla_{\boldsymbol{P}}\,\mathrm{re}\,[\boldsymbol{p}^*\boldsymbol{A}] = \frac{-\boldsymbol{kQA}}{2Q^2} \tag{31}$$

is easily derived.

5. Discussion

To an astrophysical dynamicist the KS transformation is profound, but may appear mysterious. This paper attempts to make it less mysterious, and hopefully therefore more useful, by explaining it in three-dimensional geometric terms. There are several possible directions in which the KS transformation may turn out to be useful.

First, one can imagine new orbit integrators specialized to nearly-Keplerian problems. Work on dense stellar systems with near collisions has already been mentioned (for reviews see the books Aarseth 2003; Heggie & Hut 2003). In the planetary regime, which differs from the dense-stellar case in having few bodies but many more orbital times, time transformations reminiscent of (27) used for KS regularization have proved useful for highly eccentric orbits (Mikkola 1997; Emel'yanenko 2002). Could the KS transformation itself be exploited here?

Second, it is conceivable that KS variables could simplify perturbation theory. Perturbation theory in classical celestial mechanics (see for example Murray & Dermott 2000) is algebraically frighteningly complicated, basically because the natural variables for the unperturbed and perturbed parts (being the Keplerian action-angles and real-space coordinate) are related through an implicit equation. On the other hand, the action-angles of the KS-transformed Kepler problem are explicitly related to space coordinates—the implicit equation is transferred to the time variable. Could some major simplication could be achieved through KS variables?

Third, the KS transformation might provide new insight into analogous quantum problem. (Bander & Itzykson 1966a,b) derive the symmetry groups of the bound and unbound Coulomb problem. These turn out to be the same four-dimensional symmetries as in KS theory. Is the KS transformation implicit in that work?

This work has been somewhat influenced by Scott & Frolop (2006), Follop et al. (2007),

and Miralda-Escude (2007). But only somewhat.

REFERENCES

Aarseth, S. J. 2003, Gravitational N-Body Simulations (Cambridge, UK: Cambridge University Press, November 2003.)

Aarseth, S. J. & Zare, K. 1974a, Celestial Mechanics, 10, 185

—. 1974b, Celestial Mechanics, 10, 516

Bander, M. & Itzykson, C. 1966a, Rev. Mod. Phys., 38, 330

—. 1966b, Rev. Mod. Phys., 38, 346

Bartsch, T. 2003, Journal of Physics A Mathematical General, 36, 6963

Binney, J. & Tremaine, S. 2008, Galactic dynamics (Princeton, NJ, Princeton University Press)

Emel'yanenko, V. 2002, Celestial Mechanics and Dynamical Astronomy, 84, 331

Follop, R., Rassat, A., Cooray, A., & Abdalla, F. B. 2007, astro-ph/0703806

Heggie, D. & Hut, P. 2003, The Gravitational Million-Body Problem: A Multidisciplinary Approach to Star Cluster Dynamics (The Gravitational Million-Body Problem: A Multidisciplinary Approach to Star Cluster Dynamics, by Douglas Heggie and Piet Hut. Cambridge University Press, 2003, 372 pp.)

Jernigan, J. G. & Porter, D. H. 1989, ApJS, 71, 871

Kustaanheimo, P. 1964, in Mathematische Methoden der Himmelsmechanik und Astronautik, ed. E. Stiefel, Mathematisches For- schungsinstitut Oberwolfach, Berichte 1. Bibliographisches Institut Mannheim, 330–340

Kustaanheimo, P. & Stiefel, E. 1965, J. Reine Angew. Math., 218, 204

Levi-Civita, T. 1920, Acta Math., 42, 99

Mermin, N. D. 2007, Quantum Computer Science: An Introduction (New York, NY, USA: Cambridge University Press)

Mikkola, S. 1997, Celestial Mechanics and Dynamical Astronomy, 67, 145

Mikkola, S. & Aarseth, S. J. 1989, Celestial Mechanics and Dynamical Astronomy, 47, 375

—. 1993, Celestial Mechanics and Dynamical Astronomy, 57, 439

Miralda-Escude, J. 2007, astro-ph/0703774

Murray, C. D. & Dermott, S. F. 2000, Solar System Dynamics (Cambridge, UK: Cambridge University Press, 2000.)

Scott, D. & Frolop, A. 2006, astro-ph/0604011

Stiefel, E. L. & Scheifele, G. 1971, Linear and regular celestial mechanics; perturbed two-body motion, numerical methods, canonical theory (Berlin, New York, Springer-Verlag, 1971.)

Waldvogel, J. 2006, Celestial Mechanics and Dynamical Astronomy, 95, 201